A 2-D AXISYMMETRIC CHARRING AND ABLATION
HEAT TRANSFER COMPUTER CODE

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ABSTRACT

Until recently, the capability to accomplish a two-dimensional axisymmetric nozzle thermal analysis which considers in-depth charring has not been available to the rocket nozzle analysis community except by using "pseudo" material properties to account for in-depth decomposition and using a standard 2-D axisymmetric conduction code with surface ablation.

To alleviate this problem a two-dimensional axisymmetric heat transfer and ablation computer code has been developed which accounts for in-depth decomposition. The code was developed by extensively modifying the Acurex ASTHMA II code to account for in-depth charring, grid generation and material element conductivity based upon the local element coordinate system. The code was also changed to handle as many as 2,000 elements. Code development was based on

The development of the code was based upon modeling the material response to a thermal environment in the same way as the one-dimensional Acurex CMA program. Example problems are shown to compare the charring version of ASTHMA (ASCHAR) to typical CMA models showing the resulting ablation and thermal profiles. Sample

Example problems showing the results of the ASCHAR analysis of a complete nozzle will be given showing two-dimensional thermal effects.

INTRODUCTION

Heretofore, the rocket motor design community could not adequately analyze rocket nozzles because of the lack of a 2-D axisymmetric heat transfer code which models in-depth material decomposition and the subsequent energy transport due to the pyrolysis gases percolating through the char layer to the surface. In general, most of the rocket motor community used Aerotherm's (Acurex) 1-D "Charring and Ablation Code" (CMA) to model charring. 2-D codes were available, but most of the codes which were being used did not have charring or material decomposition capabilities and as a result most of the solid rocket motor manufacturers used these noncharring codes with pseudo material properties to account for charring when 2-D analyses were required.

The disadvantages of using a noncharring 2-D code with pseudo properties are:

1. It is difficult to adequately model the properties in all temperature ranges.

2. Different heating rates cannot be accounted for, especially if at some time the cooling effects are modeled such as in post test cooling and in pulse motors when there is a nonheated coast period.

Because of the lack of an adequate tool to determine the 2-D charring effects in rocket motor nozzles, Morton Thiokol began to develop such a code in the mid-1970s. It was determined at that time that the most efficient means of developing such a code would be to modify the original Aerotherm "Axisymmetric Transient Heating and Ablation" (ASTHMA) code. The main reasons for using this code as a basis were:

1. The code was already recognized in the industry for nozzle thermal analysis expecially for nozzles with graphite and carbon/carbon throats and ITEs.

2. Heterogenous surface chemical reactions were modeled for surface ablation calculations.

Even though the ASTHMA code was a good basis to start the development of a 2-D charring code, extensive modification was required because of the following limitations.

1. Math modeling and numerical development for charring was necessary.

2. ASTHMA required that all elements (nodes) in a material had to be oriented in the same direction. (No possibility of contouring the elements with material boundaries.)

3. Original version of ASTHMA was for 200 elements maximum and as a result, a complete nozzle could not be analyzed.

4. There were limitations on applying different heating rates to many surface elements of a complete nozzle because of limitations on the number of boundary condition tables.

BACKGROUND AND THEORY

Two types of thermal analyses are generally done for estimates of temperatures and material ablation in rocket nozzles. The first is a one-dimensional analysis which is generally made for preliminary estimates of nozzle temperatures and also the prediction of the surface and indepth ablation. The analysis is completed by analyzing the nozzle at several critical locations such as the throat, nose, and exit cone.

A two-dimensional (2-D) analysis is generally made to determine the effects of irregular geometry and to obtain a detailed map of the temperatures in the nozzle so that a detailed structural analysis can be made. The scope of this paper only addresses the 2-D analysis and as a result the background and theory necessary for this type of analysis will be discussed.

The basis for the 2-D charring ASCHAR code is essentially the same as Aerotherm's (Acurex) "Charring Material Thermal Response and Ablation Program" Version 3 (CMA) except the ASCHAR is a 2-D axisymmetric code. Figure 1 illustrates the general physical problem treated by the ASCHAR code.
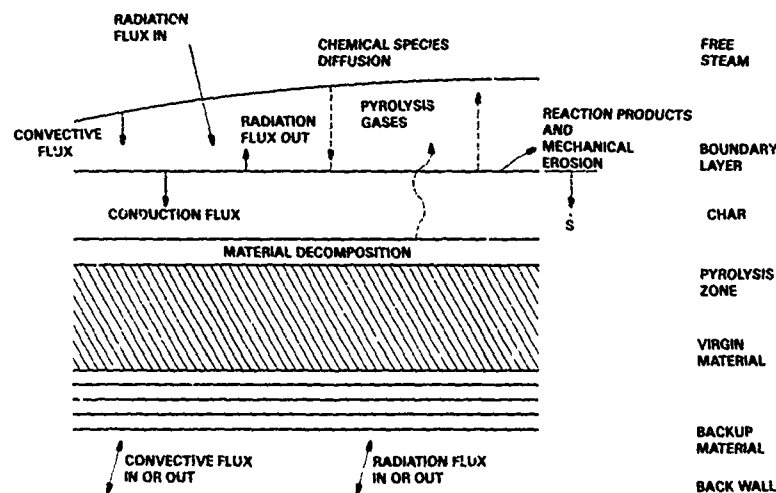

Figure 1. General Physical Problem

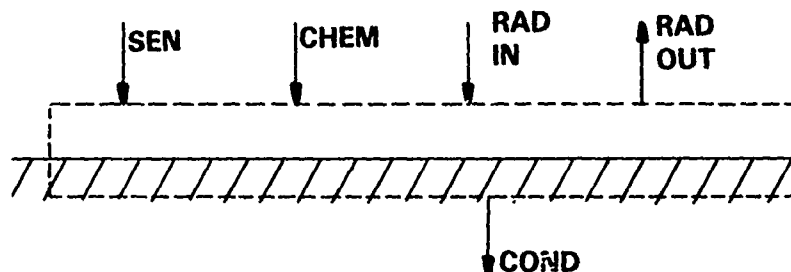The surface energy and mass balance considered by the ASCHAR code is depicted in Fig. 2.

Figure 2. Surface Energy and Mass Balance

This energy balance can by described mathematically as:

$$\underbrace{\rho_e u_e C_H (H_r - h_{ew})}_{q_{sen}} + \underbrace{\rho_e u_e C_M \ (Z^*_{iw}) h^T_i w) - B' h_w + \dot{m}_c h_c + \dot{m}_g h_g}_{q_{chem}}$$

$$+ \underbrace{\alpha_w q_{rad}}_{\substack{q_{rad} \\ \text{in}}} - \underbrace{F\alpha\varepsilon_w T^4_w - q_{cond}}_{\substack{qrad \\ \text{out}}} = 0. \tag{1}$$

where: ρ_e = local gas density at the edge conditions

u_e = local gas velocity at the edge conditions

C_H = Stanton number for heat transfer

H_r = recovery enthalpy

h_{ew} = enthalpy of the edge gas at the wall temperature

C_M = Stanton number for mass transfer

Z^*_{ie} = fraction of specie i at the edge due to chemical equilibrium and diffusion

Z^*_{iw} = fraction of specie i at the wall due to chemical equilibrium and diffusion

$h_i^T w$ = enthalpy of specie i at the wall temperature

B' = dimensionless blowing rate

$= (\dot{m}_g + \dot{m}_c)/\rho_e u_e C_M$

$\dot{m}_g$ = mass flow rate of pyrolysis gas out from surface

$\dot{m}_c$ = mass flow rate of char from surface

h_w = enthalpy of the wall gases

h_c = enthalpy of char at wall temperature

h_g = enthalpy of pyrolysis at wall temperature

α_w = surface absorptivity

q_{rad} = incident radiation flux

F = view factor

ε_w = emissivity of wall

T_w = wall temperature

q_{cond} = energy conducted into wall

The first term of equation (1) represents the sensible energy convected to the surface, the q_{chem} term represents a number of chemical energy fluxes at the surface and the remainder represents the radiation and conduction of energy to and from the wall.

The ASCHAR computer program solves the surface energy balance equation in much the same way as the original (ASTHMA II) code. However, in the indepth en~gy balance, the original version of the program does not have the capability of internal decompos..ion and the reference coordinate system is not at the wall surface. As a result no terms are associated with the pyrolysis gas leaving the surface ($\dot{m}_g h_g$) or energy transfer due to coordinate system change.

ASCHAR has this capability of indepth charring, and as a result the energy associated with gas injected into the surface control volume is necessary and a term was added to account for this energy Likewise, additional terms were added to the indepth conduction solution to account for the energy associated with decomposition and convective energy associated with pyrolysis gas moving through the material to the surface.

The equation for the indepth conduction solution is an explicit finite difference type as opposed to the implicit solution employed by CMA. The equation is:

$$
T_{m,n,\theta'} = \frac{\dfrac{T_{m+1,n,\theta}}{R_{m,n,B,\theta}} + \dfrac{T_{m,n+1,\theta}}{R_{m,n,A,\theta}} + \dfrac{T_{m-1,n,\theta}}{R_{m-1,n,B,\theta}} + \dfrac{T_{m,n-1,\theta}}{R_{m,n-1,A,\theta}} - T_{m,n,\theta}}{\dfrac{1}{R_{m,n-1,A,\theta}} + \dfrac{1}{R_{m,n,B,\theta}} + \dfrac{1}{R_{m,n,A,\theta}} + \dfrac{1}{R_{m-1,n,B,\theta}}}
$$

$$
+ \dot{M}_{pyr\ m,n,\theta}\ (H_g - \bar{H}) + \dot{M}_{m-1,n,\theta}\ \frac{dH}{dT}\ m-1,n,\theta
$$

$$
T_{m-1,n,\theta} - \dot{M}_{m,n,\theta}\ \frac{dH}{dT}\ m,n,\theta\ T_{m,n,\theta}\ \frac{\Delta\theta}{C_{m,n,\theta}} + T_{m,n,\theta}
$$

where: $T_{m,n,\theta'}$ = temperature of element m, n at the new time θ'

R = thermal resistance

A = side A of element

B = side B of element

θ = old time

$\dot{M}_{pyr\ m,n,\theta}$ = generated gas rate of element m,n

$\dot{M}_{m,n,\theta}$ = total gas rate in element m,n (generated plus gas from element m-1,n)

H_g = enthalpy of the pyrolysis gas

$\bar{H}$ = the equivalent enthalpy of the material that changes from solid to gas
defined as $(\rho_p h_p - \rho_c h_c)/(\rho_p - \rho_c)$

ρ_p = density of virgin plastic

ρ_c = density of char

h_p = enthalpy of virgin plastic

h_c = enthalpy of char

$\dfrac{dH_g}{dT}$ = slope of enthalpy vs temperature curve for pyrolysis gas

$\Delta\theta$ = time increment

C = thermal capacitance $\rho V C_p$

Note that the energy associated with the pyrolysis gas pickup is:

$$
\dot{M}_{m-1,h,\theta}\ \frac{dH}{dT}\ m-1,n,\theta\ T_{m-1,n,\theta} - \dot{M}_{m,n,\theta}\ \frac{dH}{dT}\ m,n,\theta\ T_{m,n,\theta}
$$

and the term for the material decomposition is:

$$
\dot{M}_{pyr\ m,n,\theta}\ (H_g - \bar{H})
$$

where

$$\dot{M}_{pyr\ m,n,\theta} = \sum_{j=1}^{3} \Delta\rho_j \cdot V \quad \text{and}$$

$$\Delta\rho = -B_j \exp\left(-E_j/R_t\right) \rho_{oj} \frac{(\rho_j - \rho_{rj})}{\rho_{oj}}^{\psi_j} \Delta\theta \quad (3)$$

These terms are not included in the original ASTHMA program.

Another difference between ASCHAR and ASTHMA is in the way internal thermal conductivity is treated. The basic heat conduction model employed in both programs is based upon one-dimensional flow between adjacent elements. Consequently, anisotropic heat transfer cannot be modeled exactly except in the limited case in which the axes of every element coincide with the material properties axes. However, ASCHAR provides an approximate solution when these axes do not coincide. Figure 3 shows how this is accomplished. As shown, k_1 and k_2 are the conductivities along the material major and minor axes, and θ_{AC} and θ_{BD} are the orientations of the element axes relative to the material. ASCHAR approximates the conductivity in the AC and BD directions from the following:

$$k_{AC} = k_1 \cos^2 \theta_{AC} + k_2 \sin^2 \theta_{AC} \quad (4)$$

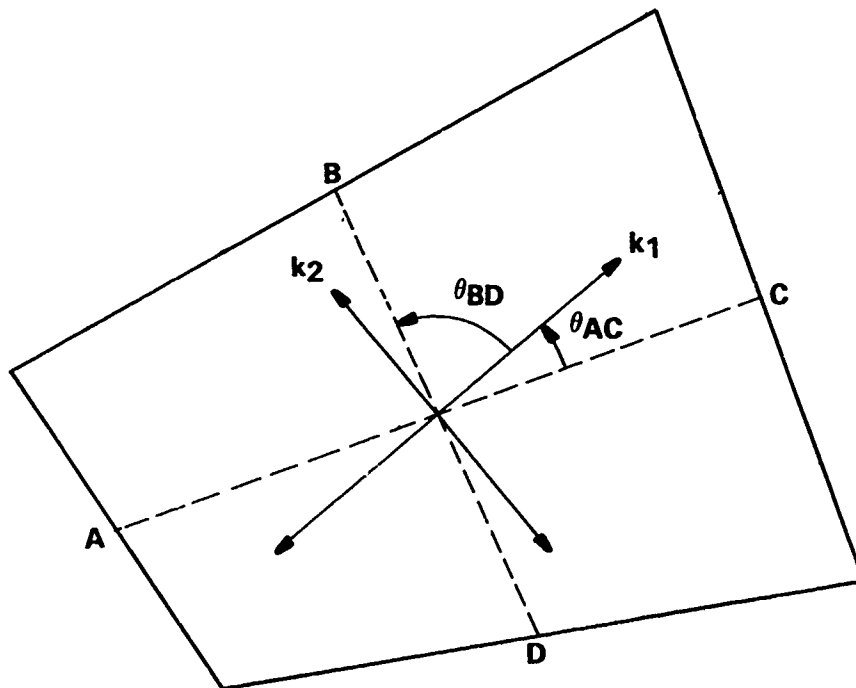$$k_{BD} = k_1 \cos^2 \theta_{BD} + k_2 \sin^2 \theta_{BD}$$

Figure 3. Material Conductivities Solution

Boundary conditions and surface thermochemistry used in the ASCHAR program are calculated by such programs as ACE or GASKET and MEIT. See References 4, 7 and 8.

ASCHAR INPUT

Basically there are four major input efforts required to run the ASCHAR program. They are the nozzle geometry, the element (node) data, the thermochemistry data and the boundary conditions. Most of the input is straight forward and the input document is all that is required.

Edge and surface thermochemistry tables are required by ASCHAR. The ACE computer code is generally used to generate this input, however other programs such as GASKET, or hand generated tables are also acceptable. Several thermochemistry tables at different pressures are selected for different locations around the nozzle as shown in Fig 4 which describes one of the example problems that was analyzed.
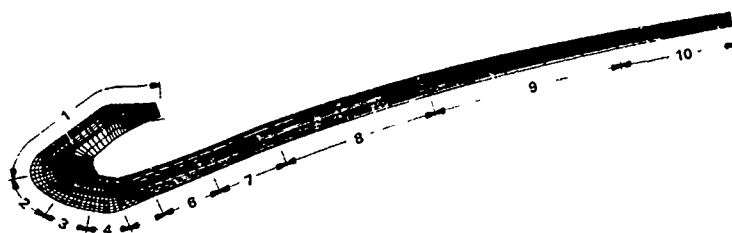
Figure 4. Strtegic Motor Nozzle Pressure Table Sections

The input for the element data or "node" data requires some discussion about the method of computing the multiplying factors for the heat transfer coefficient.

Because only a limited number of boundary condition ("function of time") tables are allowed, the program was modified to accept multiplying factors on the heat transfer coefficient so that the heat transfer coefficient could be changed from node to node in the region that applies to a particular "function of time" table. As shown in Fig. 5, there were eleven "functions of time" tables assigned to different regions of the nozzle for the carbon phenolic exit cone nozzle.
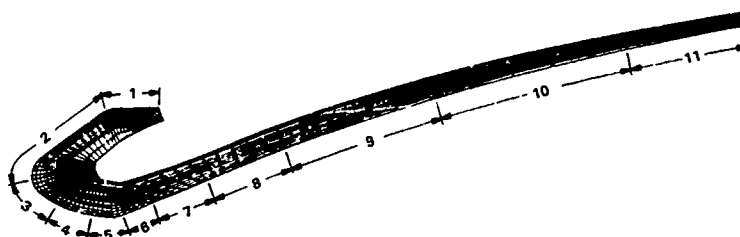
Figure 5. Strategic Motor Nozzle "Function of Time" Table Sections

The "function of time" tables used in ASCHAR are required for the recovery enthalpy, radiation flux and heat transfer coefficients. A discussion of how these variables are obtained is presented in the following paragraphs.

The recovery enthalpy is taken directly from the plot for the recovery enthalpy of MEIT output (Fig. 6).
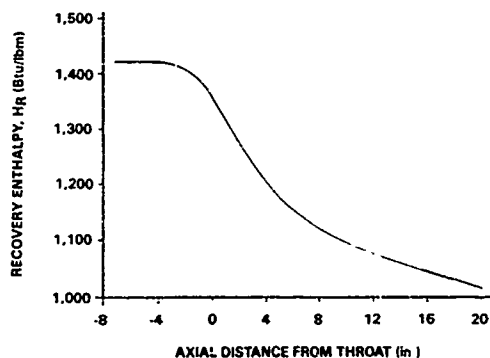
Figure 6. Carbon Phenolic Nozzle Recovery Enthalpy Distribution

The radiation input for the "function of time" tables is computed based upon the equation:

$$Q_r = \varepsilon\sigma T_s'$$

where: Q_r = incident radiation heat flux (Btu/ft^2-sec)

σ = Stefan-Boltzmann constant (4.7611 x 10^{-13} Btu/ft^2-sec-$°R^4$)

T_s = local average static temperature of combustion products (°R)

ε = emissivity of local combustion products, 1-exp [-0.808 (%Al/16) D]

%Al = percent aluminum in propellant composition
ρ = local density of combustion products including condensed species, (lbm/ft^3)

D = local nozzle diameter (in.)

The radiation flux is not generally made a function of time because the flame temperature and resulting edge temperatures do not change appreciably with pressure; therefore, the value is used as a time average value. This value is used for the entire pressure region; and, therefore, a surface node should be selected near the center of the region so that the value will represent an average value for the entire region (see **Fig. 5**).
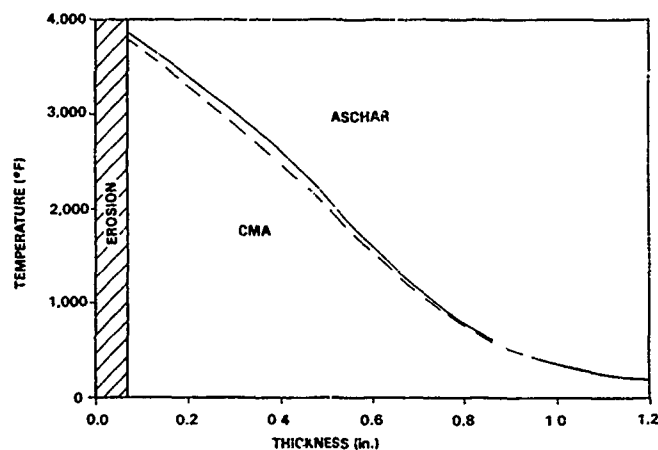

Figure 7. Comparison of ASCHAR with CMA in a Carbon Phenolic Nozzle Inlet

The heat transfer coefficient is made a function of time for a node in a particular region of the following relationship:

$$\rho_e U_e C_h, \; N \; (\theta) = \rho_e U_e C_h, \; N \; \left[\frac{P(\theta)}{\bar{P}}\right]^{0.8}$$

where: $\rho_e U_e C_h, \; N \; (\theta)$ = heat transfer coefficient of a node in a region at time θ

$\rho_e U_e C_h, \; N$ = average heat transfer coefficient of a node in a region

$P(\theta)$ = pressure at time θ

$\bar{\rho}$ = average chamber pressure

The ratio of mass transfer to heat transfer (C_m/C_h) is supposed to represent the ratio of Stanton number for mass and heat transfer. This value is approximated by:

$$\frac{C_m}{C_h} = Le^{2/3} \cong 0.7$$

However, for most materials except carbon phenolic, this factor can be used as a correlating factor to correct the "theoretical" ablation to match observed rocket motor firings. A value of C_m/C_h = 0.3 has been reasonably successful when using ACE thermochemistry for carbon/carbons similar to that used in the example nozzles (Figs.8 and 9). This value is shown in the lead card of the surface thermochemistry data which is generated by ACE.

ASCHAR VERIFICATION AND NOZZLE THERMAL ANALYSES RESULTS

To verify that the ASCHAR code is a reliable tool for nozzle thermal analysis, the code was checked by doing simple 1-D analyses using charring ablators and comparing the resulting thermal profiles with the 1-D CMA results. Figure 7 shows the results of a typical analysis and compares the 2-D ASCHAR with CMA using the same material properties and boundary conditions.

To verify that the code can actually perform complex 2-D axisymmetric nozzle thermal analysis, the results of the thermal profiles and surface ablation of three different types of nozzles as computed by the ASCHAR code are shown in Figs. 8 through 10.
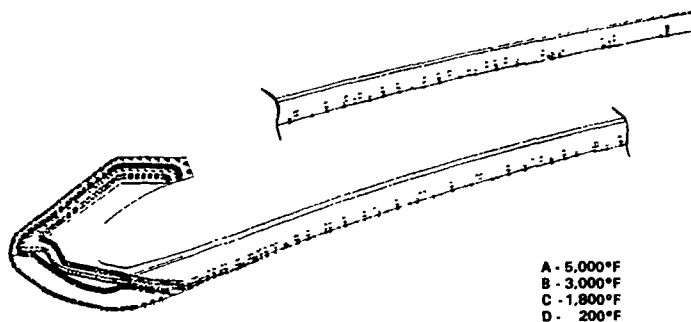

A - 5,000°F
B - 3,000°F
C - 1,800°F
D - 200°F

Figure 8. Analysis Results of Strategic Nozzle with Carbon Phenolic Exit Cone

A - 5,000°F
B - 3,000°F
C - 1,800°F
D - 500°F
E - 200°F
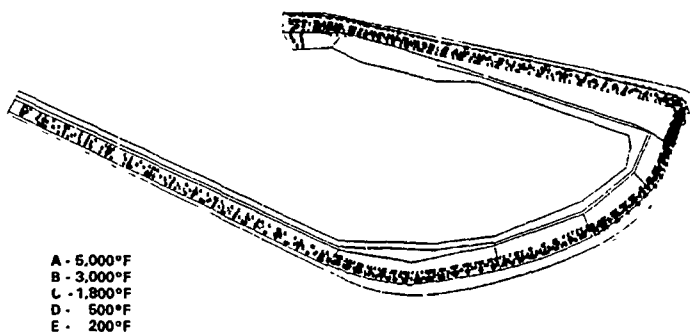
Figure 9. Analysis Results of SRM Nozzle

A - 5,000°F
B - 3,000°F
C - 1,800°F
D - 800°F
E - 200°F
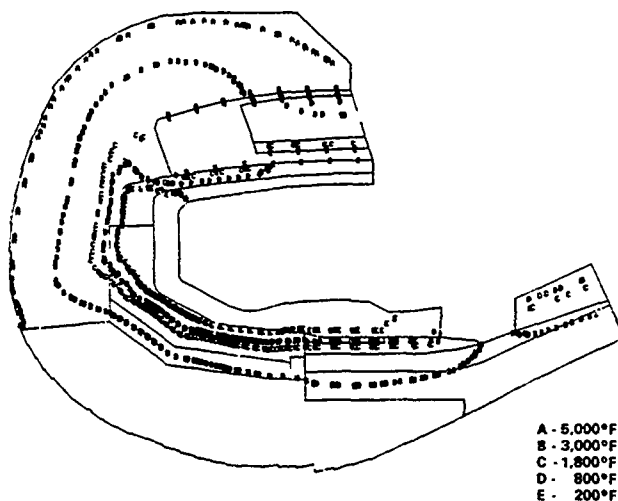
Figure 10. Analysis Results of Space Motor Nozzle

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REFERENCES

1. User's Manual - Aerotherm Charring Material Thermal Response and Ablation Program, Version 3 (CMA), AFRPL-TR-70-92.

2. User's Manual - Aerotherm Axisymmetric Transient Heating and Material Ablation Computer Program (ASTHMA 3), AFRPL-TR-72-24.

3. A User's Guide for Computer Program SEB02 - Axisymmetric Transient Heating and Ablation (ASCHAR), Morton Thiokol.

4. User's Manual - Aerotherm Chemical Equilibrium Computer Program (ACE).

5. A Computer Program for the Prediction of Solid Propellant, Motor Performance Final Report Ultra Systems, Inc. AFRPL-TR-75-36.

6. Analytical Procedure for the Thermal Response of Solid Propellant Nozzles, Aerotherm Report 75-148, U.S. Army Missile Command Propulsion Directorate, Redstone Arsenal, Alabama 35809, Contract 75-38.

7. User's Manual - Aerotherm Graphite Surface Kinetics Computer Program (GASKET 2), Aerotherm Report TR-76-13.

8   User's Manual-Aerotherm Momentum/Energy Integral Technique (MEIT), AFRPL-TR-78-53.